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Solving The Long-Standing Problem Of Low-Energy Nuclear Reactions At The Highest Microscopic Level:Annual Continuation And Progress Report

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SOLVING THE LONG-STANDING PROBLEM OF LOW-ENERGY NUCLEAR REACTIONS AT THE HIGHEST MICROSCOPIC LEVEL

ANNUAL CONTINUATION AND PROGRESS REPORT

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Background

The project "Solving the Long-Standing Problem of Low-Energy Nuclear Reactions at the Highest Microscopic Level" is an Early Career Research Program (ECRP) project funded by the Nuclear Theory Division of the Office of Nuclear Physics. Funding for this project was approved in June 2011, and became available to the PI at the beginning of August 2011. Therefore, the reporting period for Year 4 of the present project is August 15, 2014 – August 14, 2015. The present Continuation and Progress report is based on the first 7 months (August 15, 2014 – March 14, 2015) of such reporting period.

Objectives

The aim of this project is to develop a comprehensive framework that will lead to a fundamental description of both structural properties and reactions of light nuclei in terms of constituent protons and neutrons interacting through nucleon-nucleon (NN) and three-nucleon (3N) forces. This project will provide the research community with the theoretical and computational tools that will enable: (1) an accurate prediction for fusion reactions that power stars and Earth-based fusion facilities; (2) an improved description of the spectroscopy of exotic nuclei, including light Borromean systems; and (3) a fundamental understanding of the three-nucleon force in nuclear reactions and nuclei at the drip line.

To achieve this goal, we build upon a promising technique emerged recently as a candidate to reach a fundamental description of low-energy binary reactions between light ions, that is the *ab initio* no-core shell model combined with the resonating-group method (NCSM/RGM)[*,†]. This approach has demonstrated the capability to describe binary reactions below the three-body breakup threshold[‡,§] based, up to now, on similarity-renormalization-group (SRG)[**] evolved *NN* only potentials. To advance the understanding of nuclear reactions at low energies and light exotic nuclei, this project aims at extending the NCSM/RGM approach to include the full range of 3N interactions as well as the treatment of three-cluster bound and continuum states. Three-nucleon interactions are unavoidable components of a fundamental nuclear Hamiltonian obtained in a low-energy effective theory. In addition, three-nucleon force terms are induced by the SRG procedure and have to be taken into account for such a transformation to be unitary in many-body calculations. At the same time, the introduction of three-body cluster states is key to achieve a microscopic description of Borromean systems as well as three-body breakup reactions. This project will both enhance the fundamentality and enlarge the scope of our microscopic description of nuclear properties.

A successful completion of this project will result in improved accuracy of solar reaction rates and consequently, in enhancement of the predictive capability of the standard solar model. In

[*] S. Quaglioni and P. Navrátil, Phys. Rev. Lett. **101**, 092501 (2008); Phys. Rev. C **79**, 044606 (2009).
[†] P. Navrátil and S. Quaglioni, Phys. Rev. C **83**, 044609 (2011).
[‡] P. Navrátil, S. Quaglioni and R. Roth, Phys. Lett. **B704**, 379 (2011).
[§] P. Navrátil and S. Quaglioni, Phys. Rev. Lett. **108**, 042503 (2012).
[**] S. D. Glazek and K. G. Wilson, Phys. Rev. D **48**, 5863 (1993); F. Wegner, Ann. Phys. 506, 77 (1994).

addition, we will study also key reactions for the production of ^{6}Li and ^{7}Li in the standard big-bang nucleosynthesis, and the spectroscopy of Borromean halo nuclei such as ^{6}He, and ^{11}Li.

Major Goals and Objectives for the Review Period

Milestones

The milestones for the review period as described in the Year-3 Continuation and Progress Report are in part different from the Schedule and Milestones for FY2013 (Year-3) described in the original research plan given in the grant proposal, and consist in:

- Applications of recently developed NCSMC formalism and codes for the description of nucleon- and deuteron-nucleus continua with NN+3N forces:
  - First *ab initio* calculation of the ^{3}H(d,n)^{4}He and ^{3}He(d,p)^{4}He fusion reactions within the (A-1,1) + (A-2,2) + A no-core shell model with continuum using SRG-evolved NN+3N chiral EFT potentials;
- Applications of recently developed NCSM/RGM formalism and codes for the description of nucleon-nucleon-nucleus three-cluster dynamics with NN potentials:
  - Spectroscopy of ^{5}H within the ^{3}H+n+n NCSM/RGM basis using SRG-evolved NN chiral EFT potentials;
  - Spectroscopy of ^{11}Li within the ^{9}Li+n+n NCSM/RGM basis using SRG-evolved NN chiral EFT potentials;
- Implementation of the coupled (A-2,1,1) + A no-core shell model with continuum formalism and codes for the description of nucleon-nucleon-nucleus three-cluster dynamics with NN+3N forces:
  - Derivation and coding of the NN- and 3N-force couplings between (A-2,1,1) NCSM/RGM channel states and NCSM A-body eigenstates of the composite system;
  - Application to ^{4}He+n+n bound and continuum states using SRG-evolved NN+3N chiral EFT potentials;
- Implementation of (A-3,3) + A no-core shell model with continuum
  - Derivation and coding of the NN- and 3N-force couplings between (A-3,3) NCSM/RGM channel states and NCSM A-body eigenstates of the composite system;
  - Application to ^{3}H(^{3}He)+^{4}He scattering and ^{7}Li(^{7}Be) spectroscopy;
- Development of framework for the solution of the scattering problem in the presence of a binary cluster entrance channel and three-cluster exit channel

Accomplishments

No-core shell model with continuum and three-nucleon forces

A first-principle theoretical framework capable to provide a unified description of the structure and low-energy reaction properties of light nuclei is key to further refine our understanding of the fundamental nuclear interactions and providing accurate prediction of crucial reactions rates for nuclear astrophysics, fusion-energy research and other applications. However, first-principles calculations of scattering processes that account for realistic three-nucleon (3N) forces have been mostly confined to the few-nucleon sector (four nucleons or less). To address this gap in ab initio nuclear theory, as part of this project we have been developing an efficient many-body approach to nuclear bound and scattering states alike, known as the ab initio no-core shell model with continuum (NCSMC).[††,[2],[5]] In this approach, square-integrable energy eigenstates of the *A*-nucleon system are coupled to (*A*-*a*)+*a* target-plus-projectile wave functions in the spirit of the resonating group method (RGM) to obtain an efficient description of the many-body nuclear dynamics both at short and medium distances and at long ranges. Compound, target and projectile energy eigenstates are all described within the ab initio no-core shell model (NCSM). In the following we briefly review the applications of this newly developed approach completed during the past reporting period.

Predictive theory for elastic scattering and recoil of protons from helium

Personnel involved: G. Hupin (postdoc) and S. Quaglioni

Collaborators: P. Navrátil and J. Dohet-Eraly (TRIUMF)

The high fidelity of the NCSMC approach and the importance of the 3N force for the description of low-energy nuclear reactions were demonstrated in the most advanced studies of neutron (*n*) and proton (*p*) scattering on ^{4}He, using two- and three-nucleon (NN+3N) interactions derived within the framework of chiral effective field theory.[[1]] The precise and accurate results obtained for the ^{4}He(p,p)^{4}He proton elastic scattering and ^{1}H(α,p)^{4}He proton elastic recoil reactions (see Fig. 1) were particularly interesting because of the ion-beam analysis applications of these cross sections in determining the concentrations and depth profiles of helium and hydrogen, respectively, at the surface of materials or in thin films. Comparison with available experimental data showed that the NCSMC with chiral NN+3N forces constitutes a

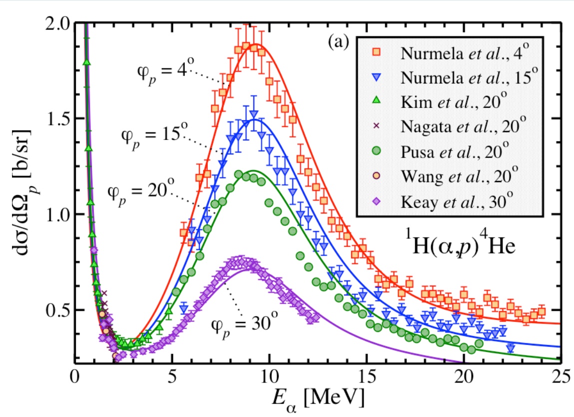

Figure 1 Calculated (solid lines) and measured (symbols) differential angular cross sections for the elastic recoil of protons by ^{4}He nuclei (or α particles) in a range of incident energies E_α and recoil angles φ_p of interest to ion-beam analyses of the concentration and depth profile of hydrogen impurities in various materials.

[††] S. Baroni, P. Navrátil and S. Quaglioni, Phys. Rev. Lett. **110**, 022505 (2013); Phys. Rev. C **87**, 034326 (2013).

predictive theory for elastic scattering and recoil of protons from helium and a competitive approach to guide applications using light-nucleus cross sections when measurements are not available. This work was published as a Rapid Communication in Physical Review C.[2]

In addition, the obtained accurate N-^{4}He scattering wave functions are currently being used as inputs for the study of the α+N bremsstrahlung,[3] the radiative process by which a photon is emitted as a result of the nuclear collision between a nucleon and a ^{4}He nucleus. This is an important study for two reasons. First, it makes possible a direct comparison between theory and experiment since α+p is one of the few light-ion systems for which bremsstrahlung cross sections were measured. Second, the α+n bremsstrahlung is a necessary preliminary step for the study of the ^{3}H(d,$n\gamma$)α bremsstrahlung cross section, which could be used to diagnose plasmas in fusion experiments but is not known well enough.

Continuum and three-nucleon force effects on the energy levels of ^{9}Be

Personnel involved: G. Hupin (postdoc) and S. Quaglioni

Collaborators: J. Langhammer, A. Calci, and Robert Roth (TU Darmstadt); P. Navrátil and A. Calci (TRIUMF)

In collaboration with J. Langhammer and Robert Roth from TU Darmstadt, the NCSMC formalism for nucleon-nucleus collisions was extended to include 3N interactions in a general framework applicable to targets heavier than ^{4}He. The extended approach allows for the assessment of effects of continuum degrees of freedom as well as of the 3N force in ab initio calculations of structure and reaction observables of p- and lower-sd-shell nuclei. The first application concerned the energy levels of the ^{9}Be system for which all excited states lie above the n-^{8}Be threshold. As can be seen in Fig. 2, for all energy levels the inclusion of the continuum significantly improved the agreement with experiment, which was an issue in standard NCSMC calculations. Furthermore, we found the proper treatment of the continuum indispensable for

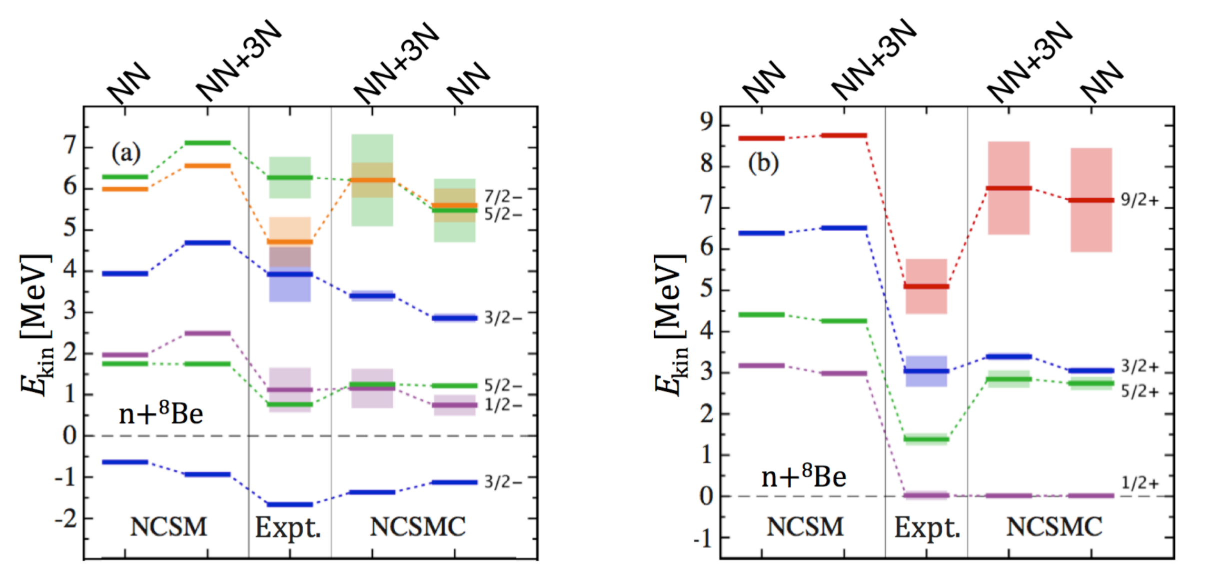

Figure 2 Computed low-lying energy spectrum of ^{9}Be (a) negative- and (b) positive-parity states compared to experiment. Here *E*kin indicates the center-of-mass energy with respect to the 8Be+*n* threshold.

reliable statements about the quality of the adopted 3N interaction from chiral effective field theory. In particular, we found the $1/2^+$ resonance energy, which is of astrophysical interest, in good agreement with experiment. This work was published as a Rapid Communication in Physical Review C.[4]

In addition, the newly developed framework is now being applied to the study of the energy levels of the ^{11}Be halo nucleus, and its photodissociation into n+^{10}Be as well as the ^{9}Be(γ,n)^{8}Be reaction.

Unified description of ^{6}Li structure and deuteron-^{4}He scattering with chiral two- and three-nucleon forces

Personnel involved: G. Hupin (postdoc) and S. Quaglioni

Collaborators: P. Navrátil (TRIUMF)

During the past reporting period we also completed and submitted to Physical Review Letters[5] the most advanced ab initio study of the ^{6}Li ground state and d-^{4}He elastic scattering. This is the most challenging and notable application of the NCSMC accomplished so far, and the first ever with the formalism to describe deuterium-nucleus collisions, which would have not been possible without the support of the present award. While ^{4}He is a fairly light target, the computational challenge in describing the d-^{4}He dynamics is related to the presence of a loosely bound composite projectile. In particular, we provided the first unified ab initio description of the ^{6}Li ground state and elastic scattering of deuterium on ^{4}He using NN+3N forces from chiral effective field theory. We analyzed the influence of the chiral 3N force and revealed the role of continuum degrees of freedom in shaping the low-lying spectrum of ^{6}Li. The calculation reproduces the empirical binding energy of ^{6}Li, yielding an asymptotic D- to S-state ratio of the ^{6}Li wave function in $d+\alpha$ configuration of −0.027 in agreement with a determination from ^{6}Li-^{4}He elastic scattering. Contrary to the lighter nuclei, this ratio was still uncertain for ^{6}Li, with different determination disagreeing even as to its sign. In addition, we used deuterium backscattering and recoil cross section data of interests to ion beam spectroscopy to validate our scattering calculations and found good agreement in particular at low energy. The

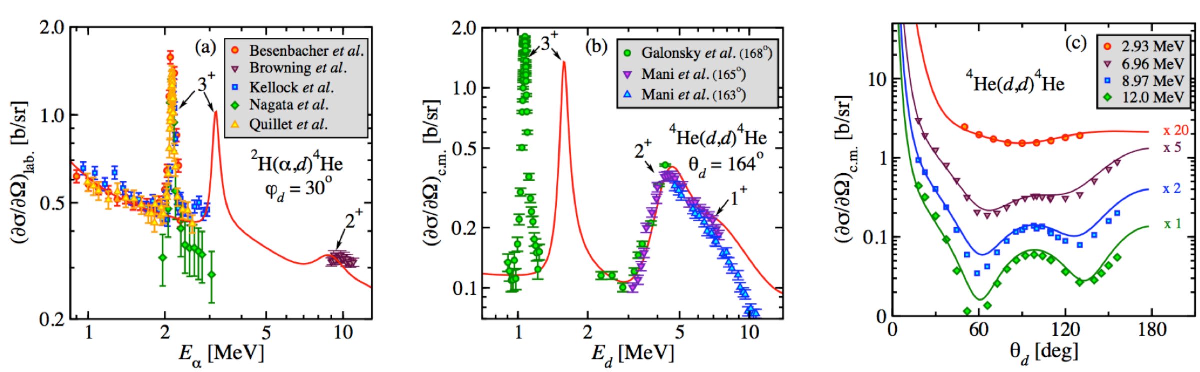

Figure 3 Computed (a) 2H(a,d)4He laboratory-frame and (b) 4He(d,d)4He center-of-mass frame angular differential cross sections (lines) using chiral NN+3N interactions as a function of the laboratory helium (E_α) and deuteron (E_d) incident energies, compared with data (symbols). In panel (c), calculated (lines) and measured (symbols) center-of-mass angular distributions at Ed = 2.93,6.96, 8.97 are scaled by a factor of 20,5,2, and 1, respectively.

overestimation by about 350 keV of the position of the 3^+ resonance, which can be seen in Figs. 3a and 3b, is an indication of remaining deficiencies of the Hamiltonian employed here. This work sets the stage for the first ab initio study of the ^{2}H(α,γ)^{6}Li radiative capture, responsible for the Big-Bang nucleosynthesis of ^{6}Li, as well as the calculation of ^{6}Li ground-state properties including the effects of the continuum degrees of freedom.

Deuterium-tritium fusion with chiral two- and three-nucleon forces

Personnel involved: G. Hupin (postdoc) and S. Quaglioni

Collaborators: P. Navrátil (TRIUMF)

The above mentioned accurate studies of nucleon- and deuterium-^{4}He elastic scattering with chiral NN+3N interactions set the stage for the most advanced ab initio calculation of the ^{3}H(d,n)^{4}He fusion, currently under way. The study is performed within an over-complete NCSMC model space including n+^{4}He and d+^{3}H continuous basis states, as well as square-integrable discrete eigenstates of the compound ^{5}He nucleus. Figure 4 shows preliminary results for the n-^{4}He scattering phase shifts from zero to 24 MeV in the center-of-mass energy. Despite the fairly small size of the harmonic oscillator basis, the calculation (performed with chiral NN+3N interactions) is in close agreement with experiment. In particular, besides a slight shift of the P-wave resonances to lower energies, the inclusion of d+^{3}H channels leads to the appearance of a resonance in the $^2D_{3/2}$ partial wave, just above the d+^{3}H threshold. This is the exit channel of the deuterium-tritium fusion. Provided the continuous availability of computing cycles, we hope to complete the calculation of the ^{3}H(d,n)^{4}He S-factor with chiral NN+3N interactions by the end of the current reporting period.

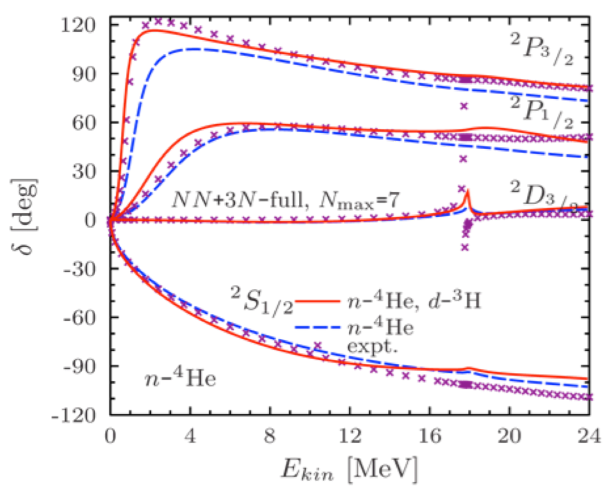

Figure 4 Preliminary results for the n-^{4}He scattering phase shifts with (solid lines) and without (dashed lines) inclusion of d-^{3}H channels as obtained in an N_{max} = 7 NCSMC model space including eigenstates of the compound ^{5}He nucleus compared to experiment.

Ab initio description of three-cluster dynamics

Nuclear systems near the drip lines, the limits of the nuclear chart beyond which neutrons or protons start dripping out of nuclei, represent a challenge for nuclear theory because of their low breakup threshold, which causes bound, resonant and scattering states to be strongly coupled. Particularly arduous in this respect are those system for which the lowest threshold for particle decay is of the three-body nature, such as ^{6}He, which decays into an alpha particle (^{4}He nucleus) and two neutrons. A rigorous description of these nuclei requires the treatment of three clusters in the continuum of energy. The same is true of nuclear reactions characterized by three-body final states, such as the ^{3}He(^{3}He,2p)^{4}He solar rate or the ^{3}H(^{3}H, 2n)^{4}He process used in diagnostics of modern fusion experiments. Therefore, Achieving an ab initio treatment of three-cluster dynamics is another important steppingstone towards gaining a basic understanding of nuclei and their reactions. In the previous reporting periods we had developed the NCSM/RGM formalism and codes to calculate bound and continuum states of three-cluster systems formed by two separate nucleons in relative motion with respect to a nucleus of mass number *A*-2, and obtained the first *ab initio* description of the ^{6}He ground state within a ^{4}He+n+n three-cluster basis. The following is a brief review of the results obtained and published since then and the progress towards including the effect of the excitations of the (*A*-2)-nucleon core.

First investigation of the ^{4}He+n+n continuum within an ab initio framework

Personnel involved: S. Quaglioni, G. Hupin (postdoc)

Collaborators: C. Romero Redondo and P. Navrátil (TRIUMF)

During the present reporting period we published in Physical Review Letters[6] the first investigation of the low-lying spectrum of the ^{6}He nucleus within an *ab initio* framework that encompasses the ^{4}He+n+n three-cluster dynamics of its lowest particle-emission channel (see Fig. 4). To bring the problem within reach of our present computational resources, for this first study we chose to work with a soft SRG-evolved NN potential (with resolution scale Λ_{SRG} = 1.5 fm^{-1}) that leads to ^{4}He ground-state energy and n+^{4}He phase shifts close to experiment despite the omission of both induced and initial chiral 3N forces. We further described the ^{4}He cluster only by its ground state and ignored core polarization effects. Working within this framework, we found the known $J^\pi = 2^+$ low-lying resonance of ^{6}He as well as results consistent with two new resonances recently observed at the SPIRAL facility of Ganil, France: a second 2^+ and a 1^+. Additional resonant states emerged in the 2^- channel near the second 2^+ resonance and in the 0^-, at slightly higher energy. On the other hand, we found no evidence of low-lying resonances but rather a broader structure in the 1^- channel. Therefore, our results do not support the idea that the accumulation of dipole strength observed at low-energy in some experiments is originated by a three-body 1^- resonance.

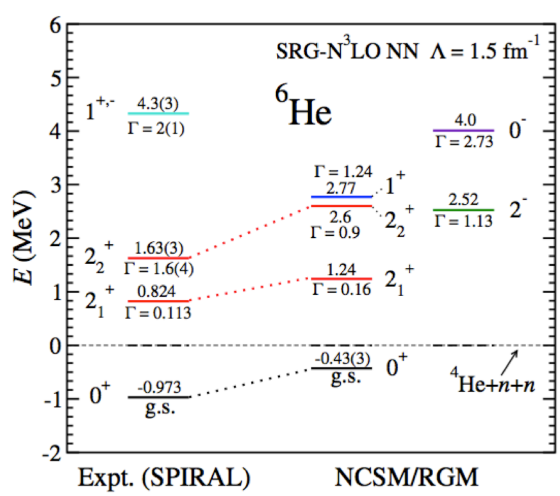

Figure 4 Low-lying energy spectrum for the ^{6}He nucleus obtained within the NCSM/RGM compared to the levels measured at the SPIRAL facility (GANIL), including the newly observed second 2^+ state. Also shown are predicted negative-parity resonances, not observed.

First investigation of the ^{3}H+n+n continuum

Personnel involved: C. Romero-Redondo (postdoc), S. Quaglioni

Collaborators: P. Navrátil (TRIUMF)

The structure of the unbound heavy hydrogen ^{5}H system is expected to be similar to that of ^{6}He, namely, a tightly bound core surrounded by two valence neutrons. The quest for ^{5}H has been undertaken in many laboratories, and, while the consensus is that it is not bound, there is presently a lively debate concerning the existence of ^{5}H as a narrow low-energy resonance. In the present reporting period we performed initial calculations of the low-lying spectrum of the ^{5}H nucleus within a ^{3}H+*n*+*n* NCSM/RGM three-cluster basis (see Fig. 5), using the same soft SRG-evolved NN interaction adopted for the study of ^{6}He. The present results point to a fairly broad $1/2^+$ ground-state resonance, but calculations in larger HO model spaces and accounting for core excitations are necessary before a definitive conclusion can be drawn on the position and width of the ^{5}H ground state.

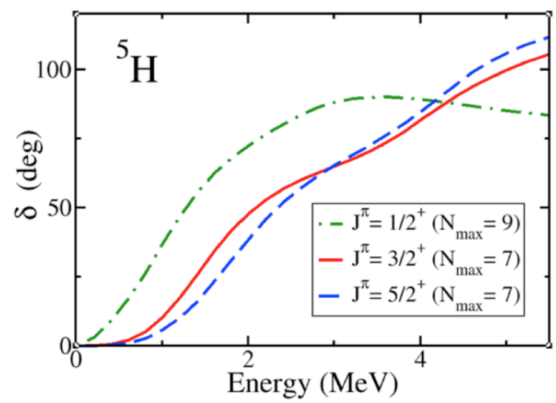

Figure 5 Preliminary results for the low-lying ^{3}H(g.s.)+n+n attractive phase shifts.

Core excitations and three-nucleon force effects in three-cluster systems

Personnel involved: C. Romero-Redondo (postdoc), S. Quaglioni

Collaborators: P. Navrátil (TRIUMF), G. Hupin (CEA/DAM)

A complete study of the low-lying spectra of the ^{6}He and ^{5}H nuclei requires still the inclusion of 3N forces and core polarization effects, both of which have been omitted for the time being. Indeed, the inclusion of explicit excited states of the core would lead to an (presently) unbearable increment of the computational size of the problem, and the situation would be worse even in the presence of 3N forces. To overcome this computational challenge, during the present reporting period we have been implementing the NCSMC approach for the description of nucleus-nucleon-nucleon dynamics by coupling the three-cluster NCSM/RGM model space with NCSM eigenstates of the composite system. In particular, we derived and implemented the required additional couplings between (*A*-2,1,1) NCSM/RGM channel states and NCSM *A*-body eigenstates of the composite system. New codes for both bound-state and continuum calculations have been already completed and are in the process of being tested. As a preliminary study we have performed calculations of the ^{6}He bound state within a an ^{4}He+n+n three-cluster basis coupled to the first square-integrable 0^+ eigenstate of ^{6}He. We adopted the same soft SRG-evolved NN interaction as in Ref. [6] and a fairly small harmonic oscillator model space of N_{tot} = 6 major shells. As expected, the obtained ground-state energy, -29.18 MeV, is lower than that from the NCSM/RGM or NCSM calculations alone by 270 keV and 1.5 MeV, respectively. The expected converged value of the ^{6}He ground-state energy for this interaction is -29.84(4) MeV. Once the testing phase will be completed, the newly developed three-cluster

NCSMC approach will be used to revisit the study of the ^{4}He+n+n and ^{3}H+n+n continua, and achieve the first ab initio description of the ^{11}Li (= ^{9}Li+n+n) low-lying spectrum. While we expect to obtain results using a soft SRG-evolved NN interaction already in the next few months, more advanced calculations including 3N forces will be completed during the next reporting period.

No-core shell model with continuum and three-nucleon projectiles

Improving the accuracy of the ^{3}H(^{3}H,2n)^{4}He and ^{3}He(α,γ)^{7}Be reaction rates, important respectively for fusion research and the standard solar model, is one of the ultimate goals of the present project. This requires the capability to describe the scattering of three-nucleon projectiles on a target.

Ab initio description of ^{3}H and ^{3}He scattering on target

Personnel involved: S. Quaglioni

Collaborators: P. Navrátil and J. Dohet-Eraly (TRIUMF), W. Horiuchi (Hokkaido University)

Initial work in this direction, namely the development of the ^{3}H/^{3}He+nucleus NCSM/RGM framework for a two-body Hamiltonian, was carried out in part under support from this grant in collaboration with W. Horiuchi and P. Navrátil.[‡‡] This formalism has now being extended by augmenting the model space with square-integrable eigenstates of the compound system, working within the NCSMC framework. Calculations of the ^{3}He(α,γ)^{7}Be and ^{3}H(α,γ)^{7}Li are currently underway and we expect that a manuscript reporting on this study will be ready by the end of the present reporting period, or soon after. Also underway is a NSCMC study of the ^{3}H-^{3}H scattering, necessary to describe the entrance channel of the ^{3}H(^{3}H,2n)^{4}He. However, we anticipate that this study, which complements the investigation of the ^{4}He+n+n exit channel discussed earlier in this document, will be completed during the next reporting period.

Operator Evolution for ab initio nuclear theory

Success in the ab initio description of light-nucleus reactions with the NCSM/RGM and NCSMC approaches has been made possible in part by the development of modern effective interaction theory, where the size of the model space required for an accurate solution of the many-body problem is substantially reduced by means of unitary transformations of the nuclear Hamiltonian. In particular, in our calculations we use similarity-renormalization group or SRG evolved two- and three-body forces. However, caution has to be taken when these interactions are used to describe, e.g., perturbation-induced reactions, where the cross section is a continuous observable depending on matrix elements of external transition operators between initial and final states. Indeed, for a fully consistent calculation the same unitary transformation applied to the Hamiltonian should be applied to any external operator. As for the Hamiltonian, this generates induced many-body terms.

[‡‡] S. Quaglioni, P. Navrátil, R. Roth, and W. Horiuchi, J. Phys.: Conf. Ser. **402**, 012037 (2012).

Evolution of scalar operators in the three-nucleon space

Personnel involved: M. D. Schuster (Summer Ph.D. Student), S. Quaglioni

Collaborators: C. W. Johnson (SDSU), E. D. Jurgneson (LLNL), and P. Navrátil (TRIUMF)

Working in a translational invariant harmonic oscillator basis for the two- and three-nucleon systems, we implemented the renormalization of external operators up to the three-body level in the framework of the SRG and studied for the first time the behavior of such renormalized three-body operators in systems with more than three nucleons, thus assessing the importance of higher-body terms. Our large-scale NCSM calculations of ^{4}He radii and total dipole strength (see Fig. 6) provided a quantitative answer to the long-sought question of how operators other than the Hamiltonian have to be treated in the context of the SRG approach. During the present reporting period, this important proof-of-principle study was published as a Rapid Communication in *Physical Review C*.[7] This work sets the stage for high-precision calculations of observables at the intersection between nuclear physics and other fields, such as the polarization of a nucleus, important in Lamb shift measurements of nuclear radii, radiative capture reactions crucial to understanding the neutrino signature of our sun, or radiative cross sections used for plasma diagnostics in fusion experiments.

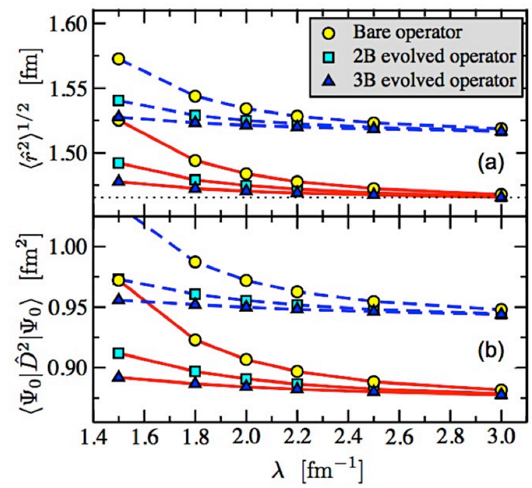

Figure 6 Calculated (a) RMS radius and (b) total dipole strength of ^{4}He as a function of SRG evolution parameter, λ. Shown are results obtained with (red solid line) and without (blue dashed line) *NNN* force, and with three levels of operator evolution: bare operator (circles), operator evolved in the two-body space (squares), and operator evolved in the three-body space (triangles). The dotted line is the RMS radius with bare Hamiltonian and bare operator.

Operator evolution for dipole transitions in ^{4}He

Personnel involved: M. D. Schuster (Summer Ph.D. Student), S. Quaglioni

Collaborators: C. Johnson (SDSU), E. D. Jurgneson (LLNL), and P. Navrátil (TRIUMF)

While the work of Ref. [7] allowed us to perform initial proof-of-principle calculations, a general description of observables also requires the ability to evolve, and embed in finite nuclei, nonscalar operators such as, e.g., the electric dipole. Further, more work is needed to accurately asses the consistency of the SRG approach for the description of continuum observables. Staring from an initial NN+3N Hamiltonian from chiral effective field theory, during the current reporting period we applied the SRG approach to compute the ^{4}He photoabsorption cross section and electric dipole polarizability. All induced forces up to the three-body level were retained in the transformed Hamiltonian, while the leading electric dipole transition operator was determined (for the first time) by evolution in the A = 2 system. All calculations were performed within the NCSM working with translational invariant harmonic oscillator (HO) basis states. The photoabsorption cross section was computed by means of the Lorentz integral

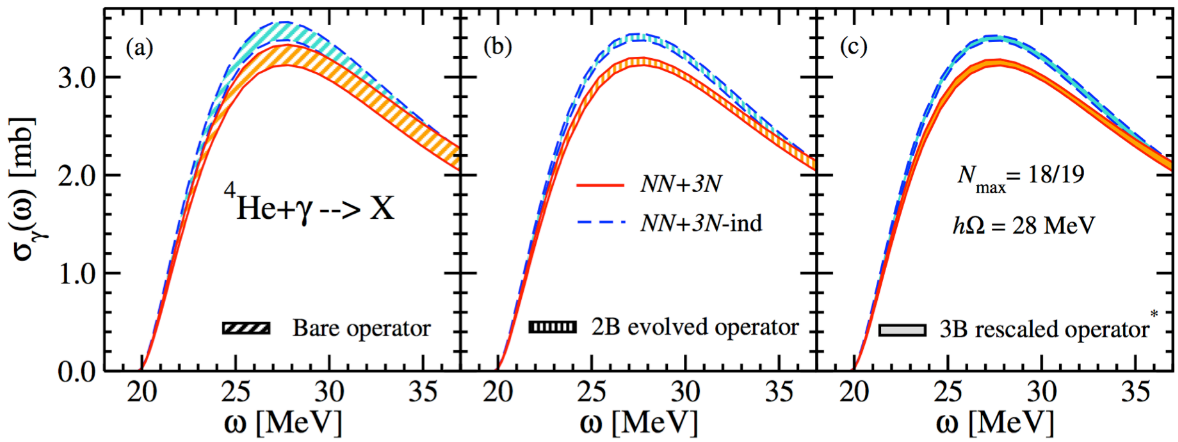

Figure 7 Dependence (represented as the width of the bands) on the variation of λ between 1.8 and 3.0 fm^{-1} of the ^{4}He photo-absorption cross section as a function of the photon energy, using the NN+3N-induced (dashed contours) and NN+3N (solid contours) wave functions. Calculations were obtained with: (a) the bare dipole operator; (b) the two-body (2B) evolved dipole operator; and (c) rescaling the 2B evolved results by the total dipole strength evolved in the three-nucleon space (3B rescaled operator*).

transform (LIT) method,[§§] while the electric polarizability is obtained using the Lanczos-moment method.[***] This techniques allowed us to bypass the direct calculation of scattering states and to work only with square-integrable basis states. As shown in Fig. 7, when using the bare dipole operator there is a clear dependence of the cross section on the SRG resolution scale λ. Further, this spread is comparable to the contribution coming from the inclusion of the initial chiral 3N force into the Hamiltonian. When we evolve the dipole operator in the two-body space, the spread in the cross section is a factor of three tighter, and the effect of the inclusion of the initial chiral 3N force can be clearly singled out. While for the time being the evolution of the non-scalar electric dipole operator has been performed only in the two-nucleoen space, three-body induced terms of the transition operator can be partly taken into account by further rescaling the cross section with the three-body evolved total dipole strength (3B rescaled operator*). The result of this operation, is mainly an overall small reduction of all curves, and a very minor narrowing of the spread in λ. The remaining dependence is due to four-body induced SRG terms and from missing three-body induced dipole operator terms. This work has been now completed and a manuscript reporting on it is in preparation and will be submitted shortly to Physical Review C.

[§§] S.Quaglioni and P.Navrátil, Phys. Lett. B **652**, 370 (2007).
[***] I. Stetcu, S. Quaglioni, J. L. Friar, A. C. Hayes, and Petr Navrátil, Phys. Rev. C **79**, 064001 (2009).

SRG resolution scale dependnce of ^{6}Li root-mean-square radius

Personnel involved: M. D. Schuster (Summer Ph.D. Student), S. Quaglioni

Collaborators: C. W. Johnson (SDSU), E. D. Jurgneson (LLNL), and P. Navrátil (TRIUMF)

Another important question concerning the SRG evolution of operators, particularly long-range ones such as the root-mean-square radius, is wheather the approximate unitary equivalence obtained in the A = 4 system through the inclusion of up to three-body induced terms is preserved in larger nuclei, , where it is computationally more advantageous to work with single-particle Slater determinant basis states. To address this issue, during the current reporting period we transformed the translationally invariant two-body evolved operators of Ref. [7] into matrix elements over Slater determinant basis states, and performed initial calculations of the resolution scale dependnce of ^{6}Li root-mean-square radius. While we have already obtained initial results working with an SRG-evolved NN interaction, more complete calculations including induced and initial 3N forces in the calculation of the ^{6}Li wave functions are still necessary for a more complete study. We anticipate that this work will be completed during the next reporting period.

Operator evolution for neutrinoless double beta decay

Personnel involved: S. Quaglioni

Collaborators: M. D. Schuster and C. W. Johnson (SDSU), J. Engel (NCU), E. D. Jurgneson (LLNL), and P. Navrátil and J. Holt (TRIUMF)

Reducing the uncertainty in the nuclear matrix elements that govern neutrinoless double-beta ($0\nu\beta\beta$) decay to well less than 50% would be a major accomplishment with important implications for the extraction of the neutrino mass scale, should $0\nu\beta\beta$ decay be observed in a near future. This would require a systematic theoretical effort extending, consistently linking, applying, and comparing several state-of-the-art techniques for light, medium-mass and heavy nuclei. An example is the effort aimed at improving shell model calculations through the use of nonperturbative effective interactions and transition operators tailored to the shell-model (SM) model space by means of Lee-Suzuky similarity transformations of ab initio coupled cluster (CC) calculations starting from SRG-evolved chiral Hamiltonians.[†††] These calculations, which for all intents and purposes can be considered ab initio SM, have already yielded promising results for nuclear energy spectra, and could lead to the first ab initio results for ^{76}Ge and ^{82}Se $0\nu\beta\beta$ decay. However, a renormalization of the $0\nu\beta\beta$ operator consistent with that applied to the nuclear Hamiltonian is necessary for the success of such a program. During the current reporting period we have initiated a collaboration with J. Engel (NCU) and J. Holt (TRIUMF) aimed at studying the effect of the SRG renormalization of $0\nu\beta\beta$ operators, using our recently developed capability to evolve non-scalar operators in the two-nucleon space. While we have already obtained preliminary results for two-body evolved matrix elements of the Gamow-Teller component of the operator, we anticipate that this study will be continued and completed during the next reporting period.

[†††] G. R. Jansen, J. Engel, G. Hagen, P. Navratil, and A. Signoracci, Phys. Rev. Lett. **113**, 142502 (2014)

Dissemination

Publications

Papers published or submitted for publication

[1] "Toward a Fundamental Understanding of Nuclear Reactions and Exotic Nuclei", S. Quaglioni, G. Hupin, J. Langhammer, C. Romero-Redondo, M. D. Schuster, C. W. Johnson, P. Navrátil, and R. Roth, JPS Conference Proceedings, in print.

[2] "Predictive Theory for Elastic Scattering and Recoil of Protons from ^{4}He", G. Hupin, S. Quaglioni, and P. Navrátil, Physical Review C **90**, 061601(R) (2014).

[3] "Microscopic Study of α+N Bremsstrahlung from Effective and Realistic Inter-nucleon Interactions", J. Dohet-Eraly, S. Quaglioni, P. Navrátil, and G. Hupin, JPS Conference Proceedings, in print (arXiv:1501.02744).

[4] "Continuum and three-nucleon force effects on ^{9}Be energy levels", J. Langhammer, P. Navrátil, S. Quaglioni, G. Hupin, A. Calci, and R. Roth, Phisycal Review C **91**, 021301(R) (2015).

[5] "Unified description of ^{6}Li structure and deuterium-^{4}He dynamics with chilar two- and three-nucleon forces", G. Hupin, S. Quaglioni, and P. Navrátil, submitted to Physical Review Letters (arXiv:1412.4101).

[6] "^{4}He+n+n continuum within an ab initio framework", C. Romero-Redondo, S. Quaglioni, P. Navrátil, and G. Hupin, Physical Review Letters **113**, 032503 (2014).

[7] "Operator evolution for ab initio theory of light nuclei", M. D. Schuster, S. Quaglioni, C. W. Johnson, E. D. Jurgenson, and P. Navrátil, Physical Review C **90**, 011301(R) (2014).

[8] "Precision measurement of the electromagnetic dipole strengths in ^{11}Be", E. Kwan et al., Physics Letters B **732**, 210 (2014).

[9] "Progress on Light-Ion Fusion Reactions with Three-Nucleon Forces", G. Hupin, S. Quaglioni, J. Langhammer, P. Navrátil, A. Calci, R. Roth, Few-Body Systems **55,** 1013 (2014).

[10] "Ab initio NCSM/RGM for three-body cluster systems and application to ^{4}He+n+n", C. Romero-Redondo, P. Navrátil, S. Quaglioni, and G. Hupin, Few-Body Systems **55,** 927 (2014).

Papers in preparation

[11] "Operator evolution for ab initio electric dipole transitions of ^{4}He", M. D. Schuster, S. Quaglioni, C. W. Johnson, E. D. Jurgenson, and P. Navrátil, in preparation.

Invited Talks

1. "Bound and continuum properties of A = 6 nuclei" by C. Romero-Redondo, Progress in Ab Initio Techniques in Nuclear Physics. February 17-20, 2015. TRIUMF, Vancouver, BC, Canada.
2. "Ab initio calculations of light-nucleus reactions and three-nucleon forces", by S. Quaglioni, Mini-Symposium on Three Nucleon Forces from Few to Heavier Nucleon Systems, 4th Joint Meeting of the APS Division of Nuclear Physics and the Physical Society of Japan, Waikoloa HI, October 7-11, 2014.
3. "Toward a fundamental understanding of nuclear reactions and exotic nuclei", by S. Quaglioni, Nuclear Structure 2014 (NS2014), Vancouver BC, July 21-25, 2014.
4. "Ab initio theory including the continuum", by S. Quaglioni, ECT* Workshop: Resonances and non-hermitian quantum mechanics in nuclear and atomic physics, ECT*, Trento, Italy, June 23-27, 2014.
5. "Toward a fundamental understanding of nuclear reactions and exotic nuclei", by S. Quaglioni, Advances in Radioactive Isotope Science 2014 (ARIS2014), Tokyo, Japan, June 1-6, 2014
6. "Present and Future Computing Requirements for Ab Initio Calculations of Nuclear Reactions and Light Exotic Nuclei", by S. Quaglioni, Large Scale Computing and Storage Requirements for Nuclear Physics (NP): Target 2017, Bethesda, MD, April 29-30, 2014

Contributed Talks

7. "Unified structure and interactions of light nuclei", by S. Quaglioni, INT 15-58W Workshop: Reactions and Structure of Exotic Nuclei, INT, Seattle, WA, March 12, 2015.
8. "Ab Initio NCSM/RGM for Three-Cluster Structure Systems", by C. Romero-Redondo, Mini-Symposium on Three Nucleon Forces from Few to Heavier Nucleon Systems, 4th Joint Meeting of the APS Division of Nuclear Physics and the Physical Society of Japan, Waikoloa HI, October 7-11, 2014.
9. "Operator evolution for ab initio theory of light nuclei", by M. D. Schuster, Mini-Symposium on Three Nucleon Forces from Few to Heavier Nucleon Systems, 4th Joint Meeting of the APS Division of Nuclear Physics and the Physical Society of Japan, Waikoloa HI, October 7-11, 2014.
10. "Three-cluster dynamics within an ab initio framework", by S. Quaglioni, INT 14-1 Program: Universaity in Few-Body Systems, INT, Seattle, WA, March 26, 2014.

Service

- Reviewer for DOE Office of Science (Nuclear Theory)
- Reviewer for NSF (Nuclear Theory)
- Member of INT National Advisory Committee
- Member of INT Director Search Committee

Additional Information

Plans for next budget period

The next will be the last budget period for this project. To meet, or at least position ourselves to meet in the immediate future, the major goals and objectives of our research activity as described in our original research plan, during the past four year we have found necessary to somewhat rethink the strategy on how best achieving the desired results, and modify (in part) the schedule of our activities and deliverables. At the same time, the more severe than anticipated computational challenges associated with the proposed work required us to rescale the scope of the project somewhat. In particular, while our initial proposal concerned the extension of the NCSM/RGM to include 3N forces and the treatment of three-cluster dynamics, practical limitations of the approach mainly related to a non-entirely efficient convergence behavior at short-to-medium distances[‡‡‡] soon made us realize that a more efficient approach was necessary to achieve the proposed improved evaluations of reaction rates for solar and Big Bang nucleosynthesis. Therefore, we increased the scope of our technical activities to include the development of the more efficient NCSMC approach. Here one works in an extended model space that, in addition to the continuous binary-cluster (A-a,a) NCSM/RGM states, encompasses also square-integrable NCSM eigenstates of the A-nucleon system. Such eigenstates introduce in the trial wave function short- and medium-range A-nucleon correlations, significantly decreasing the need for excited states of the clusters in the NCSM/RGM sector of the basis. At the same time, the NCSM/RGM cluster states provide an effective description of the tail of the wave function, and make the theory able to handle the scattering physics of the system. This change of strategy allowed us to fully meet our goals concerning the inclusion of the 3N force in the description of nucleon- and deuterium-nucleus elastic scattering,[1],[2],[4],[5] as well as ^{3}H(d,n)^{4}He transfer reaction. Further, it allowed us to achieve the first ab initio calculations of the ^{3}He(α,γ)^{7}Be and ^{3}H(α,γ)^{7}Li reaction rates, albeit without explicit 3N forces, and positioned us to obtain the first ab initio description of ^{3}H-^{3}H scattering and the three-body dynamics of two neutrons and a nuclear core, including core excitations. On the other hand, the inclusion of the 3N force and the treatment of three-cluster dynamics each proved to be far more computationally challenging than anticipated. This forced us to modify the schedule and resize the scope of the proposed applications. As of now, we expect that we will be able to deliver the proposed ab initio calculations of the low-lying spectrum of the ^{6}He with chiral NN+3N forces, but calculations including explicit 3N forces for the ^{3}He(α,γ)^{7}Be or ^{3}H(^{3}H,2n)^{4}He will likely not be achieved by the end of the next reporting period due to the explosion in number and complexity of the required NCSM/RGM kernels in the presence of a three-body projectile. Instead, we will pursue a novel approach of calculating the NCSM/RGM kernels that avoids the explicit calculation of all required permutation operators by exploiting the antisymmetrization properties of the slater determinants obtained by direct application of the relevant creation and annihilation operators on the target eigenvectors. This would alleviate the complexity of the problem, by immediately yielding the

‡‡‡ G. Hupin, J. Langhammer, P. Navrátil, S. Quaglioni, A. Calci, And R. Roth, Phys. Rev. C **88**, 054622 (2013).

sum of all required NCSM/RGM kernels. Such work will position us to achieve calculations of the ^{3}He(α,γ)^{7}Be and ^{3}H(^{3}H,2*n*)^{4}He with chiral NN+3N forces in the near future, but the development of the required parallel algorithms will be nontrivial. At the sane time, thanks to the work carried out and the computational tools developed in the past four years we will be able to accomplish unprecedented accurate calculations with chiral NN+3N forces for bound-state properties and astrophysically important reaction rates that had not been anticipated in the original proposal.

The major activities and milestones for the next (Year 5) budget period will consist in:

- Applications of the NCSMC formalism for the description of nucleon- and deuteron-nucleus dynamics with NN+3N forces:
  - First ab initio calculation of ^{4}He(N,$N'\gamma$)^{4}He bremsstrahlung;
  - Calculations of ^{6}Li ground state properties (root-mean-square radius, electric quadrupole moment, charge form factor) including the continuum degrees of freedom;
  - First ab initio calculation of the ^{2}H(α,γ)^{6}Li radiative capture;
  - Initial calculations of the ^{3}H(d,$n\gamma$)^{4}He bremsstrahlung;
- Calculations of three-cluster dynamics with core-excitation and 3N-force effects
  - Low-lying spectrum of ^{6}He within (^{4}He+n+n) + ^{6}He NCSMC model space using SRG-evolved chiral NN+3N interactions;
  - Ab initio calculation of ^{6}He ground-state properties including the continuum degrees of freedom;
  - First ab initio calculation of the ^{6}He(γ,2n)^{4}He photodissotiation
  - Low-lying spectrum of ^{5}H within (^{3}He+n+n) + ^{5}H NCSMC model space using SRG-evolved chiral NN+3N interactions;
- Calculations of ^{3}H-^{3}H and ^{3}He-^{3}He dynamics
  - Higher energy spectra of the ^{6}He and ^{6}Be nuclei within (^{3}H+^{3}H) + ^{6}He and (^{3}He+^{3}He) + ^{6}Be NCSMC model space, respectively;
  - First ab initio calculation of ^{3}H-^{3}H and ^{3}He-^{3}He scattering (the entrance channels of the ^{3}H-^{3}H and ^{3}He-^{3}He fusion, respectively);
- SRG evolution of operators
  - Study of the SRG renormalization of $0\nu\beta\beta$ operators.
  - Study of the SRG resolution scale dependence of the root-mean-square radius of ^{6}Li with chiral NN+3N forces.

Changes in personnel

Postdoctoral Researcher Guillaume Hupin left Lawrence Livermore National Laboratory on August 1st, 2014 to join a visiting scientist position oat the University of Notre Dame, waiting to start his new postdoctoral fellowship at the CEA/DAM Laboratory of Bruyères-Le-Châtel, France. Postdoctoral researcher Carolina Romero-Redondo has been hired to fill the position left vacant, and started on September 2nd, 2014. This change of personnel had some repercussions on the activities planned for the current budget period. In particular, publishing the results accumulated by Hupin became a priority, and the arrival of Romero-Redondo at the laboratory was delayed due to an unexpected lengthy process to acquire the required J1 visa.

Impact

A successful completion of this project will result in improved accuracy of the ^{3}He(α,γ)^{7}Be reaction rate and consequently, in enhancement of the predictive capability of the standard solar model. In addition, we will study also the mirror reaction ^{3}H(α,γ)^{7}Li and the ^{2}H(α,γ)^{6}Li radiative capture (respectively key reactions for the production of ^{7}Li and ^{6}Li in the standard Big-Bang nucleosynthesis), and the spectroscopy of the ^{5}H, ^{6}He, and ^{11}Li nuclei. The first ab initio calculation of the ^{6}He photodissociation and investigation of the soft-dipole excitation of this nucleus will also be achieved as part of next year project. Finally, we will study the ^{4}He($N,N'\gamma$)^{4}He and ^{3}H($d,n\gamma$)^{4}He bremsstrahlung processes and the entrance channel of the ^{3}H-^{3}H fusion, important for fusion energy research.

Participants

Project Personnel

- S. Quaglioni, PI
- G. Hupin, Postdoctoral Researcher (until August 1st, 2014)
- C. Romero-Redondo (from September 2, 2014)

External Visitors

- Postdoctoral Researcher Carolina Romero-Redondo (TRIUMF) visited Dr. Quaglioni at LLNL, supported from her home institution, from the 9 to the 19 of December 2013.

Collaborators

These collaborators contributed to our project, but were not funded by this grant:

- G. Hupin (since Aug. 2, 2014 - visiting UND)
- C. Romero-Redondo (TRIUMF, until Sep. 1, 2014)
- P. Navrátil (TRIUMF)
- A. Calci (TRIUMF)
- J. Dohet-Eraly (TRIUMF)
- R. Roth (TU Darmstadt)

- J. Langhammer (TU Darmstadt)
- C. Johnson (SDSU)
- M.D. Schuster (SDSU)
- J. Engel (NCU)
- E. Jurgenson (LLNL)